

Application of Combinatorial Chemistry to Industrial Material Problems

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Combinatorial Chemistry for Industrial Problems

- Where are the opportunities?
- What are the benefits?
- What are the high risk technical challenges?
- How can the ATP make a difference?

Opportunities & Benefits: Catalysts

<ul style="list-style-type: none">• Impacted Products<ul style="list-style-type: none">– Industrial chemicals– Engineering plastics	<ul style="list-style-type: none">• Technical Challenges<ul style="list-style-type: none">– High pressure– High temperature– Catalyst kinetics
<ul style="list-style-type: none">• Economic Benefits<ul style="list-style-type: none">– Cost reduction– Capital outlay Reduction– Speed to market– New products	<ul style="list-style-type: none">• Economic Arena<ul style="list-style-type: none">– \$375B Chemical industry– \$10B Catalyst industry– \$12B Chemical R&D

Opportunities & Benefits: Polymers

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|--|---|
| <ul style="list-style-type: none">• Impacted Products<ul style="list-style-type: none">– Engineering plastics– Commodity plastics– Plastics products | <ul style="list-style-type: none">• Technical Challenges<ul style="list-style-type: none">– Process dependent properties– Properties defined in macro terms– Scaleup issues |
| <ul style="list-style-type: none">• Economic Benefits<ul style="list-style-type: none">– Cost reduction– New products– New markets | <ul style="list-style-type: none">• Economic Arena<ul style="list-style-type: none">– \$38B plastics industry– \$1.5B polymer R&D |

Opportunities & Benefits: Phosphors

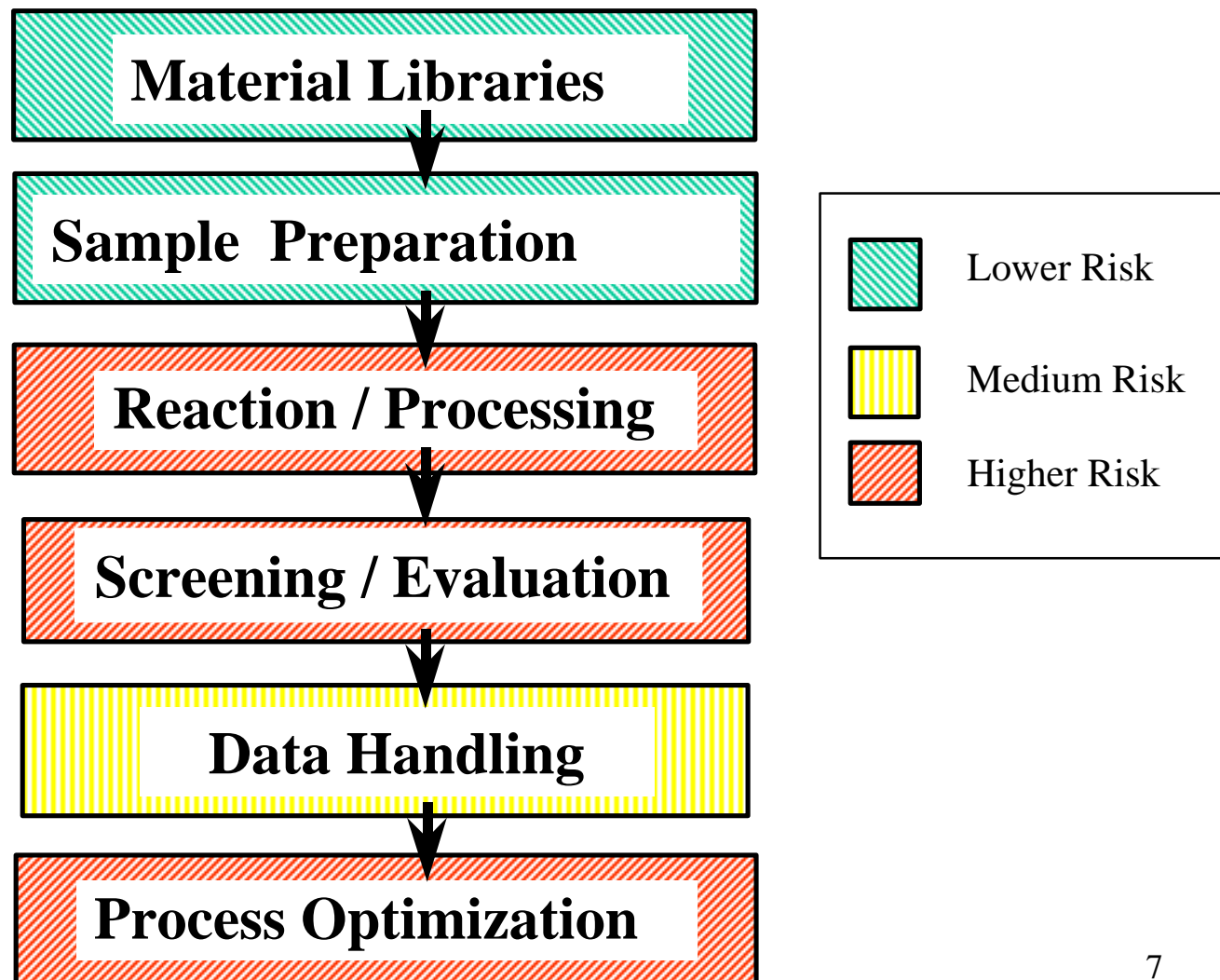
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|---|---|
| <ul style="list-style-type: none">• Impacted Products<ul style="list-style-type: none">– Domestic lighting– Automobile lighting– Electronic displays | <ul style="list-style-type: none">• Technical Challenges<ul style="list-style-type: none">– No theoretical guidance– Multispectral analysis |
| <ul style="list-style-type: none">• Economic Benefits<ul style="list-style-type: none">– Decreased energy consumption– Decreased greenhouse gases– Improved color rendition | <ul style="list-style-type: none">• Economic Arena<ul style="list-style-type: none">– Lighting consumes 25% of US electrical energy– Phosphor cost major fraction of fluorescent lamp cost |

What's Already Available?

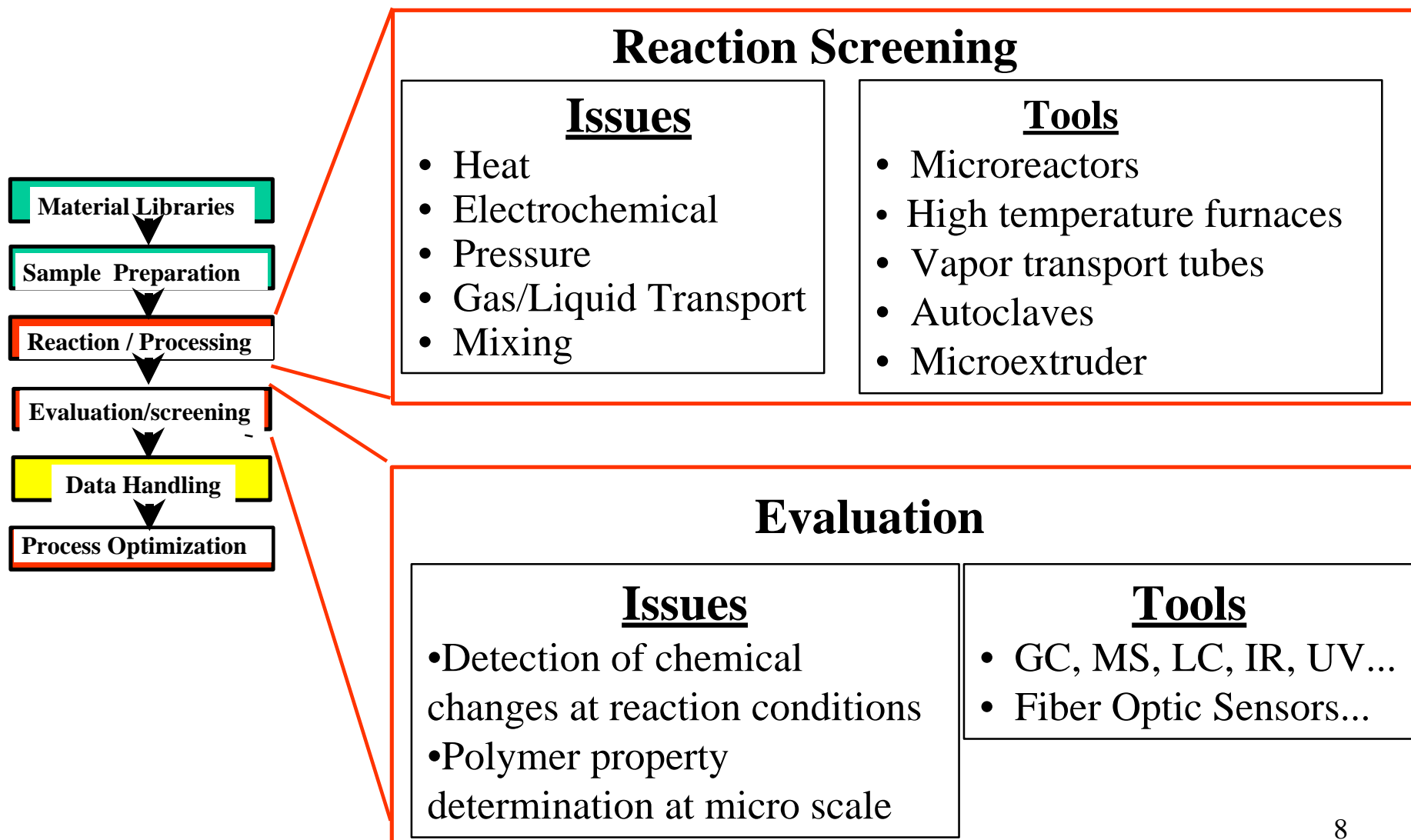
- Ideas
 - Massively parallel experimentation
 - Miniaturization of reactions and sensors
 - “Factory” organization of combinatorial experimentation
- Hardware and Software
 - Robotics
 - Analytical instruments
 - Chemical information management
 - Commercially available libraries of chemicals

(Stuff we can steal from Pharmaceutical research!)

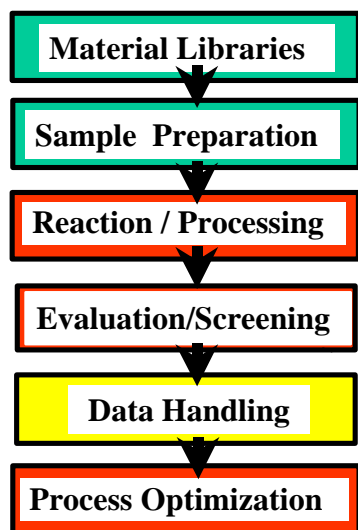
Challenges: Technique Development



High Risk Technical Challenges



High Risk Technical Challenges



• Issues

- Reactor miniaturization
- Sampling
- Scaleup
- Multiple reactor types
- Detection

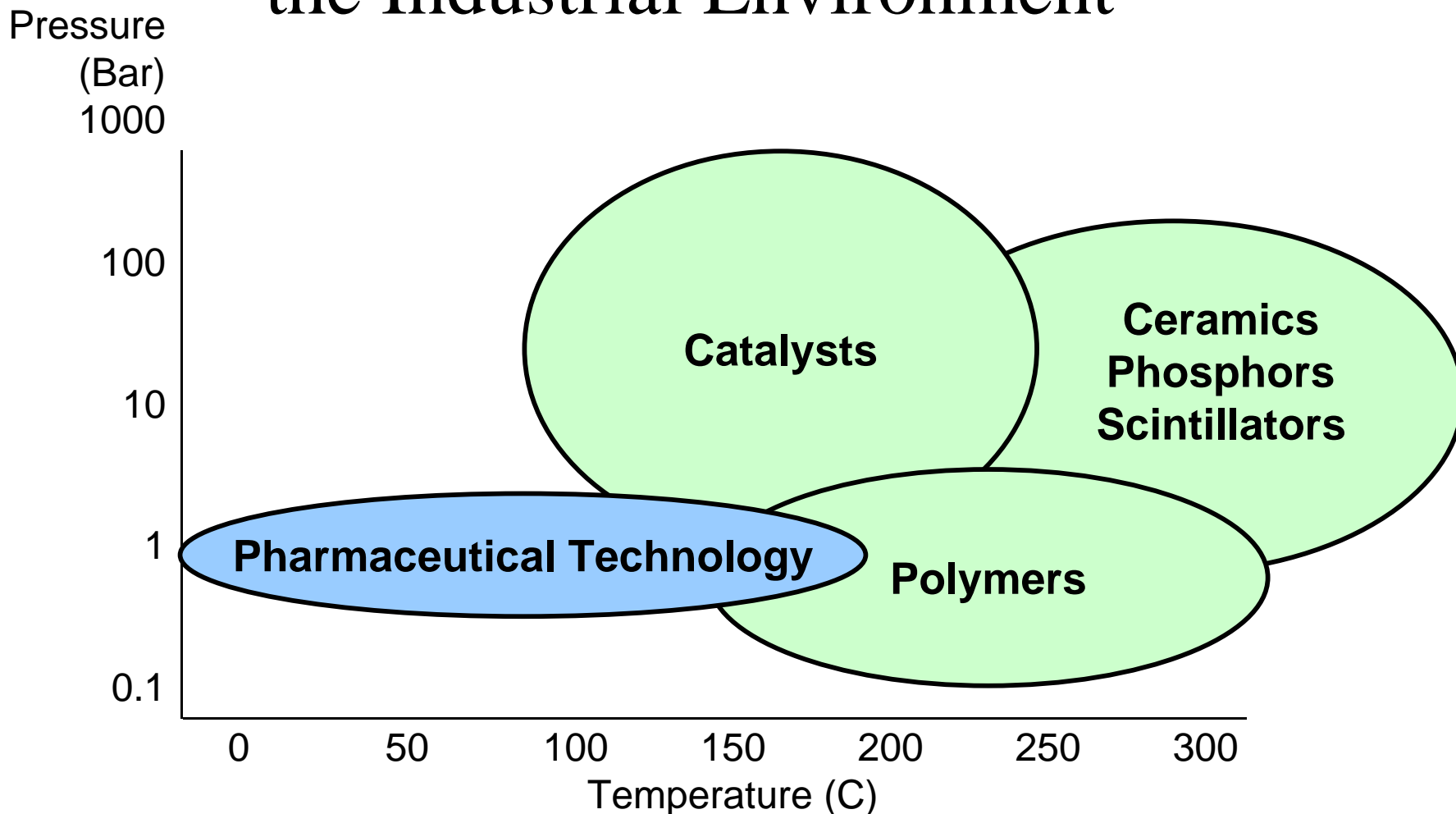
• Reactors

- Continuous Flow
- High Pressure
- High Temperature
- Tubular
- Back-Mixed
- Heterogeneous
- Extruders

• Sensors

- Continuous
- Within the vessel
- Chemical properties
- Physical properties
- Surface properties
- Optical properties
- Mechanical properties

High Risk Technical Challenges: the Industrial Environment



Technical Issues to be Tackled with ATP Support

- Miniaturization of reaction, processing, and testing apparatus
- Clear understanding of “scalability”
- Generally useful high throughput synthetic or fabrication methods
- Generally useful high throughput measurement and screening technology

The ATP Opportunity

- Jump start combinatorial infrastructure
 - Develop versatile combinatorial technology
 - Reduce capital intensity of combinatorial systems
- Reduce the barriers to entry
 - Achieve and publicize industrial combinatorial successes
 - Reduce cultural barriers to changing from “solo inventor” to “research factory”

Meet the global technical challenge